Perturbative-Nonperturbative Duality: Nonperturbative method for quantum mechanics

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Abstract

Quantum mechanical perturbation theory encounters two difficulties: (1) For systems with densely spaced high-energy levels (e.g., the Coulomb potential), a perturbation theory that works for low-energy levels fails for high-energy levels. (2) For systems with scattering states (also, e.g., the Coulomb potential), even for low-energy levels like the ground state, the perturbation theory encounters highly challenging integrals over scattering states. The first difficulty invalidates perturbation theory, while the second complicates its application. This paper proposes a method to overcome these difficulties, based on the generalization of the Newton-Hooke duality and the discovery of duality families. Using the duality relation, we construct a dual system for the target system—one without dense energy levels or scattering states—making it suitable for perturbation theory. After calculating the eigenvalues of the dual system by standard perturbation theory, we obtain the eigenvalues of the target system through the duality transformation.

Contents

1 Introduction

Difficulties in the stationary perturbation theory. Approximation methods are essential in quantum mechanics, as exact solutions are generally unavailable except for a few special cases. Perturbation theory is one of the most widely used approximation methods. However, it encounters difficulties when energy levels are densely spaced. This paper proposes a solution for applying perturbation theory to systems with densely spaced energy levels. Our approach involves constructing a *non-dense*-energy-level system dual to the original *dense*-energy-level system of interest. Here, "duality" refers to the relationship where the solutions of the two systems are interconnected via a duality transformation. Since the dual system's energy levels are not densely spaced, standard perturbation theory can be applied. Finally, through the duality relationship, we transform the perturbative solution of the dual system into a nonperturbative solution of the dense-energy-level system, for which conventional perturbation theory fails.

Typically, dense energy levels are encountered in the following two situations.

1. The low-lying energy levels are not dense, but the high-lying ones are dense, such as in the Coulomb potential (Figure 1). In this case, perturbation theory does not apply to high-lying energy levels. The condition for the Hamiltonian

$$H = H_0 + H' \tag{1}$$

to be amenable to perturbation theory is

$$\left|\frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}\right| \ll 1. \tag{2}$$

Here, the perturbation matrix element $H'_{mn} = \left\langle \psi_m^{(0)} \right| H' \left| \psi_n^{(0)} \right\rangle$, where the zeroth-order eigenvalue $E_n^{(0)}$ and eigenvector $\left| \psi_n^{(0)} \right\rangle$ are determined by the eigenequation $H_0 \left| \psi_n^{(0)} \right\rangle = E_n^{(0)} \left| \psi_n^{(0)} \right\rangle$. In cases where energy levels are dense at high-energy states, even if the spacing between low-energy levels exceeds the perturbation strength, i.e., $\left| E_n^{(0)} - E_m^{(0)} \right| > \left| H'_{mn} \right|$, allowing perturbation theory to be valid for low-energy states, the spacing at high-energy states may become smaller than the perturbation, leading to the failure of perturbation theory for high-energy states. In such cases, for a given perturbation H', low-energy states can be treated perturbatively, whereas high-energy states require nonperturbative methods, implying that perturbation theory applies only to the low-energy states. Conversely, in cases like the harmonic oscillator potential, where all energy levels are non-dense, perturbation theory remains applicable to all energy levels.

2. Both bound states and scattering states exist, such as in the Coulomb potential (as shown in Figure 1). The energy levels of the scattering states are continuous and, of course, dense. In this case, even if we only calculate the perturbation of the non-dense low-energy states, we inevitably encounter difficulties brought by the dense energy levels of the high-energy states. This is because, taking the second-order correction as an example, the perturbation correction involves both a sum over discrete bound-state energy levels and an integral over continuous scattering-state energy levels:

$$E_n^{(2)} = \sum_{m \neq 0} \frac{H'_{nm}}{E_n^{(0)} - E_m^{(0)}} + \int d\mathrm{k} \frac{H'_{n\mathrm{k}}}{E_n^{(0)} - E_\mathrm{k}^{(0)}}. \tag{3}$$

The integral over the scattering states is often very difficult, and usually only the upper and lower bounds of the correction can be estimated [1]. More precise treatment requires special techniques, such as the Sternheimer method [2,3], the parabolic coordinate method [4], the

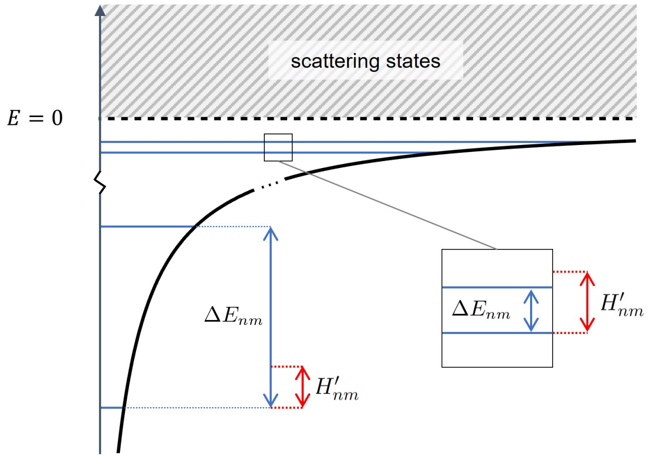

Figure 1: The Coulomb potential: non-dense low-lying energy levels, dense high-lying energy levels, and continuous spectral scattering states.

Dalgarno-Lewis method [5], and the steepest descent method [6]. In contrast, the harmonic oscillator potential possesses only bound states with entirely discrete energy levels, thus avoiding the difficulties arising from the integral over continuous spectra.

We use the Coulomb potential as an example because it features both densely spaced high-energy bound states and continuous scattering states. Consequently, perturbative calculations will encounter both difficulties mentioned above: the nonperturbative issue arising from dense energy levels and the continuous spectrum integral encountered in all second-order and higher-order perturbation calculations.

Duality. The method proposed in this paper is to transform potentials, such as the Coulomb potential, which are unsuitable for perturbation theory due to their dense energy levels and/or continuous-spectral scattering states, into potentials like the harmonic oscillator with non-dense energy levels and no scattering states, which are suitable for perturbation theory. Our method is based on a duality concept proposed by Newton [7]. In *Principia*, Newton revealed a duality between the gravitational potential and the harmonic oscillator potential, now known as the Newton-Hooke duality. Later, the Newton-Hooke duality was generalized to arbitrary power-law potentials in classical mechanics, known as the Kasner-Arnol'd theorem [8,9]. The orbits of two dual potentials, i.e., the solutions to their equations of motion, can be transformed into each other through a duality transformation. By solving for the orbit of one dual potential, the orbit of the other can be obtained via this duality transformation. This inspired us to transform a nonperturbative problem into a perturbative one by finding, for a potential unsuitable for perturbation theory, a dual potential that is suitable. This method essentially transforms a nonperturbative problem into a solvable perturbative problem.

The Newton-Hooke duality provides a transformation that preserves the type of equations of motion. Compare the duality transformation with the symmetry transformation: under a symmetry transformation, the equation remains unchanged, while under a duality transformation, the equation type remains unchanged, but the equation itself transforms into another equation. In physics, a duality transformation transforms the equation of motion into another equation of the same type: a Newtonian equation with different forces [7–10], a scalar field equation with a different self-interaction potential [10], a Schrödinger equation with a different potential [10, 11], a nonlinear Schrödinger equation with different nonlinear terms [11], a Gross-Pitaevskii equation with different nonlinear terms and potentials [12], a generalized KdV equation with different nonlinear coefficients in the first-order derivative term [13], and so forth.

A recent discovery regarding the Newton-Hooke-type duality inspires an indirect method for solving equations of motion. This discovery reveals that the Newton-Hooke-type duality is not limited to pairwise systems; rather, a duality family exists [10]. A duality family contains an infinite number of members that are dual to each other. This means that what is dual to universal gravitation is not limited to the harmonic oscillator; rather, there are infinitely many mechanical systems dual to universal gravitation, and all these mutually dual systems constitute a duality family. One only needs to solve one member of the duality family, and the solutions of all other members can be obtained through the duality transformation. The indirect approach based on the duality family is to first identify the duality family containing the target equation, then solve an easy-to-solve member of the family, and finally apply the duality transformation to obtain the solutions for all family members, including, of course, the original target equation [14–17]. The nonperturbative method proposed in this paper is an indirect method based on the duality family. Previously, such indirect methods were only used to find exact solutions, whereas this paper combines this duality-based indirect method with perturbation theory to propose a nonperturbative method.

The example considered in this paper is the Coulomb potential. As mentioned earlier, the high-energy states of the Coulomb potential are essentially nonperturbative, and for low-energy states, second-order and higher-order perturbations encounter difficult-to-handle integrals over scattering states. Our approach is to first find an easy-to-handle dual potential for the Coulomb potential. The Coulomb potential has infinitely many dual potentials, and we choose the harmonic oscillator potential (which corresponds to the Newton-Hooke duality in classical mechanics). The harmonic oscillator potential has only bound states, all energy levels are non-dense, and there are no scattering states, making it ideal for perturbation theory. After obtaining the perturbative solution for the harmonic oscillator using standard perturbation theory, we apply a duality transformation to convert this solution into a nonperturbative solution for the Coulomb potential. In essence, the duality here is a perturbative-nonperturbative duality.

Rydberg atoms, which are atoms in highly excited states, have important applications in fields such as quantum information, quantum computing [18–20], quantum optics [21–23], and quantum simulation [24–32]. Although the example in this paper is the hydrogen atom, Rydberg atoms are hydrogen-like in nature; for instance, the Rydberg states of many atoms, such as rubidium and cesium, behave very similarly to those of hydrogen. In these atoms, the excited electron has a very large orbital radius and is far from the atomic nucleus. For such highly excited states, even a very weak external field cannot be treated as a perturbation. Therefore, the method presented in this paper can be naturally applied to these Rydberg atoms.

In section 2, we outline the method. In section 3, we illustrate the method with an example. In section 4, we present our conclusions.

2 Duality-based nonperturbative method

Technically, the method proposed in this paper requires transforming a perturbative series into the nonperturbative solution of its dual potential through a duality transformation. This section presents the duality transformation for the series solution. The result is for the spherically symmetric power-law potential, but this method is generally developed.

The eigenfunctions and eigenvalues of two dual potentials are related through a duality transformation [10]. However, the eigenvalue given by the duality transformation is an implicit expression [15], making it technically challenging to obtain an explicit expression for the nonperturbative eigenvalue from the perturbative series solution of its dual system. This section provides an explicit expression for the nonperturbative eigenvalue.

2.1 Duality: brief review

In Ref. [10], we presented the duality relation for two spherically symmetric potentials.

The stationary Schrödinger equations for spherically symmetric potentials $U(r)$ *and* $V(\rho)$*,*

$$\begin{aligned} \frac{d^2u_l(r)}{dr^2}+\left[E-\frac{l(l+1)}{r^2}-U(r)\right]u_l(r) &= 0, \quad (4)\\ \frac{d^2v_\ell(\rho)}{d\rho^2}+\left[\mathcal{E}-\frac{\ell(\ell+1)}{\rho^2}-V(\rho)\right]v_\ell(\rho) &= 0, \quad (5)\end{aligned}$$

if they satisfy

$$\frac{r^2}{\left(l+\frac{1}{2}\right)^2}\left[U(r)-E\right]=\frac{\rho^2}{\left(\ell+\frac{1}{2}\right)^2}\left[V(\rho)-\mathcal{E}\right], \quad (6)$$

with

$$r\longleftrightarrow\rho^\sigma, \quad (7)$$

then their solutions are related by the duality transformation

$$u_l(r)\longleftrightarrow\rho^{(\sigma-1)/2}v_\ell(\rho). \quad (8)$$

The angular momentum of the dual system is

$$l+\frac{1}{2}\longleftrightarrow\frac{1}{\sigma}\left(\ell+\frac{1}{2}\right). \quad (9)$$

It is noteworthy in this dual transformation that σ is an arbitrary constant; different values of σ yield different dual potentials. Selecting an easy-to-solve family member from the duality family, obtained by taking all possible values of σ, and then using the duality transformation to obtain solutions for the rest of the family members, constitutes an indirect method for solving the equation [14, 15].

This paper uses polynomial-type central potentials as an example, but the method also applies to potentials of other forms.

From the duality relation, it follows that the relationship between two polynomial-type central potentials

$$\begin{aligned} U(r) &= \xi r^a+\mu r^b, \quad (10)\\ V(\rho) &= \eta\rho^A+\lambda\rho^B, \quad (11)\end{aligned}$$

is

$$\begin{aligned} \sigma &= \frac{A+2}{2}=\frac{2}{a+2}, \quad (12)\\ (b+2)\sigma &= B+2, \quad (13)\end{aligned}$$

$$\begin{aligned} \mathcal{E} &\longleftrightarrow -\sigma^2\xi, \quad (14)\\ \eta &\longleftrightarrow -\sigma^2 E, \quad (15)\\ \lambda &\longleftrightarrow \sigma^2\mu. \quad (16)\end{aligned}$$

If the eigenvalue of the potential $U(r)$ is

$$E = E(n_r, \xi, \mu, l), \tag{17}$$

where n_r is the radial quantum number, then the eigenvalue of the dual potential is

$$\mathcal{E} = -\sigma^2 E^{-1}\left(n_r, -\frac{\eta}{\sigma^2}, \frac{\lambda}{\sigma^2}, \frac{1}{\sigma}\left(\ell+\frac{1}{2}\right)-\frac{1}{2}\right). \tag{18}$$

Here, E^{-1} denotes the inverse function.

2.2 Duality transformation of series solution

Perturbation theory provides a series solution, while the duality transformation yields a solution in implicit functions (18), which is difficult to apply in practice. To address this, we present a duality transformation for the series solution with an explicit expression.

Suppose the potential to be solved is

$$V(\rho) = V_0(\rho) + \lambda V_I(\rho), \tag{19}$$

where λ is *not* small, rendering perturbation theory inapplicable.

According to the duality relation in section 2, we construct a perturbative system dual to the potential $V(\rho)$:

$$U(r) = U_0(r) + \mu U_I(r). \tag{20}$$

Here, $U_0(r)$ is also dual to $V_0(\rho)$, and μ is small; hence, the potential $U(r)$ is suitable for perturbation theory. Using standard perturbation theory, we can obtain a perturbative series for the eigenvalues for the dual potential $U(r)$,

$$E = E^{(0)} + \mu E^{(1)} + \mu^2 E^{(2)} + \cdots. \tag{21}$$

The perturbative corrections at each order are given by [33]

$$E_n^{(k)} = \sum_{n=1, m\neq n} \frac{K(k-1, m, n)}{E_n^{(0)} - E_m^{(0)}} H'_{nm}, \; k > 1, \tag{22}$$

where $K(k, m, n) = E_n^{(k)} - \sum_{j=1}^{k-1} E_n^{(j)} \frac{K(k-j,m,n)}{E_n^{(0)}-E_m^{(0)}}$.

Our method is nonperturbative. We utilize the duality transformation to obtain a nonperturbative approximation for the potential $V(\rho)$ from the perturbative solution of its dual potential $U(r)$, Eq. (21). Technically, this requires finding the inverse function of a series

$$\mathcal{E} = -\sigma^2 \textsc{InverseFunction}\left(E^{(0)} + \mu E^{(1)} + \mu^2 E^{(2)} + \cdots\right). \tag{23}$$

To avoid confusion with the reciprocal notation, we use $\textsc{InverseFunction}(f(x))$ to denote the inverse of $f(x)$, rather than $f^{-1}(x)$. We express the eigenvalue $\mathcal{E}$ as a series

$$\mathcal{E} = \mathcal{E}^{(0)} + \mathcal{E}^{(1)}\lambda + \mathcal{E}^{(2)}\lambda^2 + \cdots; \tag{24}$$

note that since λ is not small, this series is not a perturbative series.

We next solve (23) for the eigenvalue $\mathcal{E}$, which is given in implicit form.

Substituting the duality relations (16) and (15) into (21) yields

$$\frac{1}{\sigma^2}\eta + \sum_{n=0}\left(\frac{1}{\sigma^2}\lambda\right)^n E^{(n)}[\mathcal{E}(\lambda)] = 0, \tag{25}$$

and Taylor expanding $E^{(n)}\left(\mathcal{E}\left(\lambda\right)\right)$ yields

$$E^{(n)}\left(\mathcal{E}\left(\lambda\right)\right)=\sum_{k=0}\frac{1}{k!}\left.\frac{d^{k}E^{(n)}\left(\mathcal{E}\left(\lambda\right)\right)}{d\lambda^{k}}\right|_{\lambda=0}\lambda^{k}. \tag{26}$$

By applying the Faà di Bruno formula [34],

$$\frac{d^{n}}{dx^{n}}f(g(x))=\sum_{k=1}^{n}f^{(k)}(g(x))B_{n,k}\left(g'(x),g''(x),\ldots,g^{(n-k+1)}(x)\right), \tag{27}$$

where $B_{n,k}$ is the Bell polynomial, given in recurrence form as

$$B_{n+1,k+1}\left(x_{1},\cdots,x_{n-k+1}\right)=\sum_{i=0}^{n-k}\begin{pmatrix} n \\ i \end{pmatrix}x_{i+1}B_{n-i,k}\left(x_{1},\cdots,x_{n-i-k+1}\right) \tag{28}$$

with $B_{0,0}=1$ and $B_{n,k}\big|_{n<k}=0$ [35], or, equivalently,

$$B_{n,k}\left(x_{1},\cdots,x_{n-k+1}\right)=\sum_{l_{1}+2l_{2}+\ldots+(n-k+1)l_{n-k+1}=n}\frac{n!}{l_{1}!\cdots l_{n-k+1}!}\prod_{j=1}^{n-k+1}\left(\frac{x_{j}}{j!}\right)^{l_{j}}, \tag{29}$$

where $k=l_{1}+l_{2}+\cdots+l_{n-k+1}$, where the summation runs over all integer partitions satisfying $l_{1}+2l_{2}+\ldots+(n-k+1)l_{n-k+1}=n$ [36–39], and from (24), we have $\left.\frac{d^{r}\mathcal{E}(\lambda)}{d\lambda^{r}}\right|_{\lambda=0}=r!\mathcal{E}^{(r)}$, we then arrive at

$$\left.\frac{d^{k}E^{(n)}\left(\mathcal{E}\left(\lambda\right)\right)}{d\lambda^{k}}\right|_{\lambda=0}=\sum_{l=0}^{k}\frac{d^{l}E^{(n)}\left(\mathcal{E}\left(\lambda\right)\right)}{d\mathcal{E}\left(\lambda\right)^{l}}B_{k,l}\left(1!\mathcal{E}^{(1)},2!\mathcal{E}^{(2)},\cdots,(k-l+1)!\mathcal{E}^{(k-l+1)}\right). \tag{30}$$

Substituting into (25) and utilizing the Cauchy product formula, $\left(\sum_{i=0}^{\infty}a_{i}\right)\left(\sum_{i=0}^{\infty}b_{i}\right)=\sum_{i=0}^{\infty}\sum_{j=0}^{i}a_{j}b_{i-j}$, we obtain

$$\frac{1}{\sigma^{2}}\eta+\sum_{n=0}^{\infty}\sum_{j=0}^{n}\sum_{k=0}^{n-j}\frac{1}{\sigma^{2j}}\frac{1}{(n-j)!}\left.\frac{d^{k}E^{(j)}\left(\mathcal{E}\right)}{d\mathcal{E}^{k}}\right|_{\mathcal{E}=\mathcal{E}^{(0)}}B_{n-j,k}\left(1!\mathcal{E}^{(1)},2!\mathcal{E}^{(2)},\cdots,(n-j-k+1)!\mathcal{E}^{(n-j-k+1)}\right)\lambda^{n}=0. \tag{31}$$

Equating the coefficients of each power of λ to zero yields the equations for $\mathcal{E}^{(n)}$.

Zeroth-order approximation:

$$\frac{1}{\sigma^{2}}\eta+E^{(0)}\left(\mathcal{E}^{(0)}\right)=0, \tag{32}$$

hence

$$\mathcal{E}^{(0)}=-\sigma^{2}\textsc{InverseFunction}\left[E^{(0)}\right]. \tag{33}$$

Higher-order corrections obey the following recurrence relation,

$$\sum_{j=0}^{n}\sum_{k=0}^{n-j}\frac{1}{(n-j)!\sigma^{2j}}\left.\frac{d^{k}E^{(j)}\left(\mathcal{E}\right)}{d\mathcal{E}^{k}}\right|_{\mathcal{E}=\mathcal{E}^{(0)}}B_{n-j,k}\left(1!\mathcal{E}^{(1)},2!\mathcal{E}^{(2)},\cdots,(n-j-k+1)!\mathcal{E}^{(n-j-k+1)}\right)=0. \tag{34}$$

In the Bell polynomial $B_{n,k}\left(\cdots,x_{n-k+1}\right)$, since $B_{n,1}=x_{n}$ and $B_{n,0}=0$, only terms containing x_{n} and no terms with x_{n+1} can appear, so (34) is a linear equation in $\mathcal{E}^{(n)}$. Rewriting (34) as

$$\mathcal{E}^{(n)}\left.\frac{dE^{(0)}\left(\mathcal{E}\right)}{d\mathcal{E}}\right|_{\mathcal{E}=\mathcal{E}^{(0)}}+\sum_{j=0}^{n}\sum_{k=0,k\neq1}^{n-j}\frac{1}{(n-j)!\sigma^{2j}}\left.\frac{d^{k}E^{(j)}\left(\mathcal{E}\right)}{d\mathcal{E}^{k}}\right|_{\mathcal{E}=\mathcal{E}^{(0)}}B_{n-j,k}\left(1!\mathcal{E}^{(1)},\ldots,(n-1)!\mathcal{E}^{(n-1)}\right)=0, \tag{35}$$

we have

$$\mathcal{E}^{(n)} = -\frac{1}{\left.\frac{dE^{(0)}(\mathcal{E})}{d\mathcal{E}}\right|_{\mathcal{E}=\mathcal{E}^{(0)}}} \sum_{j=0}^{n}\sum_{k=0,k\neq 1}^{n-j} \frac{1}{(n-j)!\sigma^{2j}} \left.\frac{d^k E^{(j)}(\mathcal{E})}{d\mathcal{E}^k}\right|_{\mathcal{E}=\mathcal{E}^{(0)}} B_{n-j,k}\left(1!\mathcal{E}^{(1)},\cdots,(n-1)!\mathcal{E}^{(n-1)}\right). \tag{36}$$

This recursive relation for $\mathcal{E}^{(n)}$ can be solved order by order.

3 Perturbative hydrogen atom: example

3.1 Nonperturbative problem of dense high-energy-state energy level

Due to dense high-energy-state levels and scattering states, both difficulties mentioned in the introduction are simultaneously encountered when applying perturbation theory to the hydrogen atom. Therefore, the perturbation problem for hydrogen atoms serves as an ideal test case for our proposed method.

Consider the hydrogen atom system with perturbation $-\frac{\lambda}{\rho^2}$,

$$\frac{d^2 v_\ell(\rho)}{d\rho^2} + \left\{\left[\mathcal{E} - \frac{\ell(\ell+1)}{\rho^2} - \frac{\eta}{\rho}\right] - \frac{\lambda}{\rho^2}\right\} v_\ell(\rho) = 0. \tag{37}$$

To validate our method, we select an example with a known exact solution: the exact eigenvalue is $\mathcal{E} = -\frac{\eta^2}{\left(1+2n_r+\sqrt{(2\ell+1)^2+4\lambda}\right)^2}$.

According to the method proposed in this paper, the first step is to find a dual system for this perturbed hydrogen atom system. This dual system should (1) lack dense energy levels and (2) lack scattering states, thereby overcoming the two difficulties encountered in applying perturbation theory to the hydrogen atom.

There are infinitely many systems dual to (37), and we choose the three-dimensional spherically symmetric harmonic oscillator perturbed by $-\frac{\mu}{r^2}$,

$$\frac{d^2 u_l(r)}{dr^2} + \left\{\left[E - \frac{l(l+1)}{r^2} - \xi r^2\right] - \frac{\mu}{r^2}\right\} u_l(r) = 0. \tag{38}$$

which has non-dense energy levels and no scattering states. The duality relation between these two systems is

$$\begin{aligned} E &\longleftrightarrow -4\eta, \\ \xi &\longleftrightarrow -4\mathcal{E}, \\ l+\frac{1}{2} &\longleftrightarrow 2\left(\ell+\frac{1}{2}\right), \\ \mu &\longleftrightarrow 4\lambda. \end{aligned} \tag{39}$$

From (36), we can obtain the perturbation series for the eigenvalues of the perturbed harmonic oscillator (38):

$$E_{n_r l} = \left[(3+2l+4n_r) + \frac{2}{2l+1}\mu - \frac{2}{(2l+1)^3}\mu^2 + \frac{4}{(2l+1)^5}\mu^3 + \cdots\right]\sqrt{\xi}. \tag{40}$$

This result is consistent with that obtained by directly expanding the exact eigenvalue

$$E = \left(4n_r + 2 + \sqrt{(2l+1)^2 + 4\mu}\right)\sqrt{\xi}. \tag{41}$$

Following the recursive relation (36), we obtain the eigenvalues of the required perturbed hydrogen atom system

$$\begin{aligned}\mathcal{E}_{n_r\ell} &= -\frac{\eta^2}{4\left(n_r+\ell+1\right)^2}+\frac{\eta^2}{2\left(n_r+\ell+1\right)^3\left(2\ell+1\right)}\lambda-\frac{\left(2n_r+8\ell+5\right)\eta^2}{4\left(n_r+\ell+1\right)^4\left(2\ell+1\right)^3}\lambda^2\\ &+\frac{\left(2n_r^2+16\ell^2+7n_r+10n_r\ell+21\ell+7\right)\eta^2}{2\left(n_r+\ell+1\right)^5\left(2\ell+1\right)^5}\lambda^3+\cdots. \end{aligned}\tag{42}$$

This result is also consistent with that obtained by directly expanding the exact eigenvalue $\mathcal{E}=-\frac{\eta^2}{\left(1+2n_r+\sqrt{(2\ell+1)^2+4\lambda}\right)^2}$.

The above results demonstrate the validity of our method.

Let us do some order-of-magnitude analysis.

Between two highly excited states $n_r=100\ell=20$ and $n_r=99\ell=20$, i.e., $\Delta n_r=1$ and $\Delta\ell=0$, the perturbation matrix element is

$$\mathcal{H}'=\int v_{100,20}^{(0)*}\left(\rho\right)\frac{\lambda}{\rho^2}v_{99,20}^{(0)}\left(\rho\right)d\rho=5.1782\times10^7\eta^2\lambda,\tag{43}$$

while the difference between these two states is

$$\Delta\mathcal{E}^{(0)}=\mathcal{E}_{100,20}^{(0)}-\mathcal{E}_{99,20}^{(0)}=2.85775\times10^{-7}\eta^2.\tag{44}$$

The ratio of the perturbation matrix element to the energy level interval is

$$\left|\frac{\mathcal{H}'}{\Delta\mathcal{E}^{(0)}}\right|\sim1.81199\times10^{14}\lambda.\tag{45}$$

This clearly shows that even for small λ, the ratio generally becomes large, indicating that perturbation theory does not apply to high-excited hydrogen atom states. In contrast, for the harmonic oscillator dual to the above hydrogen atom, the ratio is

$$\left|\frac{H'}{\Delta E^{(0)}}\right|\sim5.13507\times10^{-3}\mu=2.05403\times10^{-2}\lambda.\tag{46}$$

This implies that the nonperturbative problem of a hydrogen atom becomes a perturbative problem after being duality-transformed into a harmonic oscillator.

It should be noted that we treat the two radial equations (37) and (38) as two one-dimensional problems, so there is no degeneracy, and non-degenerate perturbation theory can be used. The accuracy of the obtained results also confirms this point.

3.2 Integral over scattering state

The hydrogen atom possesses both a discrete spectrum of bound states ($\mathcal{E}<0$) and a continuous spectrum of scattering states ($\mathcal{E}>0$). Therefore, even for the ground state, the second-order correction encounters the difficulty of integrating over scattering states. By (3), the second-order correction for the perturbed hydrogen atom (37) is $\mathcal{E}_n^{(2)}=\sum_{m\neq0}\frac{\mathcal{H}'_{nm}}{\mathcal{E}_n^{(0)}-\mathcal{E}_m^{(0)}}+\int\frac{\mathcal{H}'_{n\mathrm{k}}}{\mathcal{E}_n^{(0)}-\mathcal{E}_\mathrm{k}^{(0)}}d\mathrm{k}$. The summation part of the second-order correction for the ground state ($n_r=0$ and $\ell=0$) is

$$\sum_{m_r\neq0}\frac{\mathcal{H}_{0m_r}^2}{\mathcal{E}_0-\mathcal{E}_{m_r}}=-\sum_{m_r=1}^{\infty}\frac{\left[\frac{1-\left(\frac{m_r}{m_r+2}\right)^{m_r+1}}{2(m_r+1)^{3/2}}\eta^2\lambda\right]^2}{-\frac{\eta^2}{4}-\left(-\frac{\eta^2}{4(m_r+1)^2}\right)}\sim-0.195001\eta^2\lambda^2.\tag{47}$$

However, the exact second-order contribution obtained by expanding the exact solution of the eigenvalue differs significantly, being

$$\mathcal{E}_0^{(2)\text{Exact}} = -\frac{5\eta^2\lambda^2}{4} = -1.25\eta^2\lambda^2, \tag{48}$$

indicating a substantial contribution from the scattering states.

In contrast, the harmonic oscillator, the dual potential of the hydrogen atom, has only discrete bound-state eigenvalues, avoiding the difficulty of scattering-state integrals, yielding

$$E_0^{(2)} = \sum_{m_r \neq 0} \frac{H_{0m_r}^2}{E_0 - E_{m_r}} = -\sum_{m_r=1}^{\infty} \frac{1}{4m_r(1+m_r)}\mu^2\sqrt{\xi} = -\frac{\mu^2\sqrt{\xi}}{4}.$$

4 Conclusion

This paper proposes a duality-based approach to address two challenges in the stationary perturbation theory of quantum mechanics: the nonperturbative problem in systems with dense high-excited state energy levels and the scattering-state integral in systems with scattering states.

Both issues involve dense energy levels. Our method is to find, for these systems with dense energy levels and/or scattering states, a dual system that has non-dense energy levels and no scattering states, thereby eliminating the two difficulties mentioned above.

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